Ground state fidelity in bond-alternative Ising chains with Dzyaloshinskii-Moriya interactions

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A systematic analysis is performed for quantum phase transitions in a bond-alternative one-dimensional Ising model with a Dzyaloshinskii-Moriya (DM) interaction by using the fidelity of ground state wave functions based on the infinite matrix product states algorithm. For an antiferromagnetic phase, the fidelity per lattice site exhibits a bifurcation, which shows spontaneous symmetry breaking in the system. A critical DM interaction is inversely proportional to an alternating exchange coupling strength for a quantum phase transition. Further, a finite-entanglement scaling of von Neumann entropy with respect to truncation dimensions gives a central charge $c \simeq 0.5$ at the critical point.

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I. INTRODUCTION

Recent advanced material technologies have made it possible to access low-dimensional quantum systems. Furthermore, material synthesis has offered a great opportunity to explore more intriguing lower-dimensional spin systems rather than well-understood conventional spin systems [1]. In such a low-dimensional system, for instance, alternating bond interactions and/or less symmetry interactions in spin lattices can be realizable in synthesizing two different magnetic atoms. Of particular importance, therefore, is understanding quantum phase transitions in which one-dimensional spin systems are unlikely found naturally.

Normally, quantum fluctuations in a low-dimensional spin system are stronger than higher dimensional spin systems [2]. Quantum phase transitions driven by stronger quantum fluctuations then exhibit more interesting and novel quantum phenomena in low-dimensional spin systems. The effects of alternating bond interactions, especially, have been intensively studied theoretically in spin systems such as antiferromagnetic Heisenberg chains [3–8], Heisenberg chains with next-nearest-neighbor bond alternations [9, 10], a tetrameric Heisenberg antiferromagnetic chain [11], and two-leg spin ladders [12, 13]. A recent experiment has demonstrated a realization of a bond-alternating chain by applying magnetic fields in a spin-1/2 chain antiferromagnet [14].

In this study, we will consider one-dimensional Ising-type spin chains with an alternating exchange coupling. Actually, this bond alternation cannot destroy the antiferromagnetic phase of the uniform bond case but just quantitatively changes the ground state properties originating from a dimerization of the spin lattice. Then, a less symmetric interaction can play a significant role to induce a quantum phase transition. To see a quantum phase transition, we will employ a Dzyaloshinskii-Moriya (DM) interaction [15] which results from the spin-orbit coupling.

Based on the ground state fidelity [16] with the iMPS presentation [17], we discuss the quantum criticality in the system. It is shown that a uniform DM interaction can destroy the antiferromagnetic phase, which is a continuous quantum phase transition, and its critical value is inversely proportional to the alternating exchange coupling strength.

II. MODEL AND NUMERICAL METHOD

Let us start with a spin-1/2 Ising chain with antisymmetric anisotropic, and alternative bond interactions on the infinite-size lattice. Our system can be described by the spin Hamiltonian

$$H = \sum_{i=\infty}^{\infty} J_i S_i^z S_{i+1}^z + \vec{D}_i \cdot (\vec{S}_i \times \vec{S}_{i+1}), \qquad (1)$$

where $\vec{S}_i = (S_i^x, S_i^y, S_i^z)$ are the spin operators acting on the i-th site. The exchange interaction is chosen as $J_i = 1 - (-1)^i r$ and the alternative bond interaction is characterized by the relative strength r of exchange coupling for the even and odd lattice sites. To describe an antisymmetric anisotropic exchange coupling between the two spins on the lattice, we employ a uniform DM interaction $\vec{D}_i = \vec{D}$, that is characterized by the DM vector $\vec{D} = (D_x, D_y, D_z)$. For $r = 0$ and $\vec{D} = 0$, Eq. (1) is reduced to the conventional Ising chain Hamiltonian. If $r = 0$ and $\vec{D} = D\hat{z}$, Eq. (1) can be mapped onto the XXZ spin chain model which has a quantum phase transition from the gapped Neel or antiferromagnetic (AFM) phase to the gapless Luttinger Liquid (LL) phase at the critical point $D_c = 1$ [20]. This study will then be focused on the antiferromagnetic exchange interaction $J_i \geq 0$, i.e.,

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$0 \leqslant r \leqslant 1$, and a transverse DM interaction denoting $\vec{D} = (0, 0, D)$.

The Hamiltonian in Eq. (1) is actually invariant under the transformation $U = \prod U_{2i} \otimes U_{2i+1}$ with $U_{2i} = \sigma^x$ for $2i$-th site and $U_{2i+1} = \sigma^y$ for $(2i+1)$-th site. Our model Hamiltonian then possesses a Z_2 symmetry generated by the transformation U. The ground state of the system may undergo a spontaneous Z_2 symmetry breaking which gives rise to a quantum phase transition between an ordered phase and a disordered phase.

For a quantum spin system with a finite N lattice site, its wave function with the periodic boundary condition can be expressed in the matrix product state (MPS) representation [18] as $|\Psi\rangle = \mathrm{Tr}\left[A^{[1]}A^{[2]}\cdots A^{[N]}\right]|s^{[1]}s^{[2]}\cdots s^{[N]}\rangle$, where $A^{[i]}$ is a site-dependent $\chi \times \chi$ matrix with the truncation dimension χ of the local Hilbert space at the i-th site, $|s^{[i]}\rangle$ is a basis of the local Hilbert space at the i-th site, and the physical index s takes value $1, \cdots, d$ with the dimension d of the local Hilbert space. This MPS representation for a finite lattice system can be extended to describe an infinite lattice system. To do this, for an infinite lattice, one may replace the matrix $A^{[i]}$ with $\Gamma^{[i]}\lambda^{[i]}$ [17], where $\Gamma^{[i]}$ is a three-index tensor and $\lambda^{[i]}$ is a diagonal matrix at the i-th site, which is called the *canonical infinite matrix product state* (iMPS) representation.

If system Hamiltonian is translational invariant for an infinite lattice, for instance, our system Hamiltonian describe by Eq. (1) has a two-site translational invariance, the two-site translational invariance allows us to reexpress the Hamiltonian as $H = \Sigma_i h^{[i,i+1]}$, where $h^{[i,i+1]}$ is the nearest-neighbor two-body Hamiltonian density. In such a case, one can introduce a two-site translational invariant iMPS representation, i.e., for the even (odd) sites A (B), only two three-index tensors $\Gamma_{A(B)}$ and two diagonal matrices $\lambda_{A(B)}$ can be applied in representing a system wave function:

$$|\Psi\rangle = \sum_{\{s^{[i]}\}} \cdots \Gamma_A\lambda_A\Gamma_B\lambda_B\Gamma_A\lambda_A\Gamma_B\lambda_B\cdots|\cdots s^{[i]}s^{[i+1]}s^{[i+2]}s^{[i+3]}\cdots\rangle. \tag{2}$$

Note that, actually, for an infinite lattice sites, the diagonal elements of the matrix λ_i are the normalized Schmidt decomposition coefficients of the bipartition between the semi-infinite chains $L(-\infty, ..., i)$ and $R(i+1, ..., \infty)$.

In order to find a ground state of our system in the iMPS representation, the infinite time-evolving block decimation (iTEBD) algorithm introduced by Vidal [17] is employed. For a given initial state $|\Psi(0)\rangle$ and the Hamiltonian H, a ground-state wave function can be yield by the imaginary time evolution $|\Psi(\tau)\rangle = \exp\left[-H\tau\right]|\Psi(0)\rangle/|\exp(-H\tau)|\Psi(0)\rangle|$ for a large enough τ. To realize the imaginary time evolution operation numerically, the imaginary time τ is divided into the time slices $\delta\tau = \tau/N$ and a sequence of the time slice evolution gates approximates the continuous time evolution. Meanwhile, the time evolution operator $\exp\left[-h^{[i,i+1]}\delta\tau\right]$ for $\delta\tau \ll 1$ is expanded to a product of the evolution operators acting on two successive i and $i+1$ sites through the Suzuki-Trotter decomposition [19]. After absorbing a time-slice evolution gate, in order to recover the iMPS representation, a singular value decomposition of a matrix is performed, which contracted from Γ_A, Γ_B, one λ_A , two λ_B and the evolution operators. Then only the χ largest singular values are retained. This procedure yields the new tensors Γ_A, Γ_B and λ_A that are used to update the tensors for all the sites. As a result, the translational invariance under two-site shifts is recovered. Repeating the above procedure until the ground-state energy converges yields the ground-state wave function of the system in the iMPS representation.

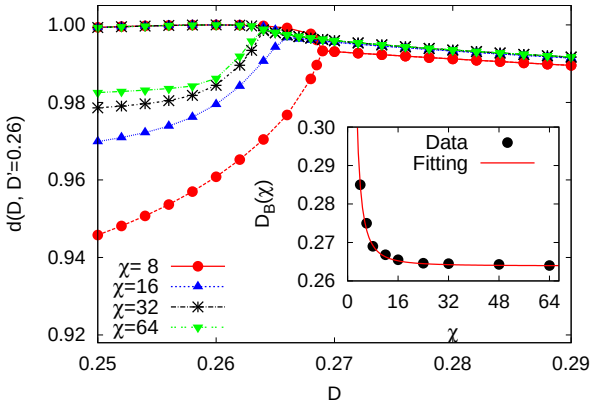

FIG. 1: (Color online) Fidelity per lattice site $d(D, D' = 0.26)$ as a function of D for various truncation dimensions χ with $r = 0.5$. For higher truncation dimension, a bifurcation point $D_B(\chi)$ moves to saturate to its critical value. Inset: Extrapolation of bifurcation point $D_B(\chi)$. From the numerical fitting function $D_B(\chi) = D_B(\infty) + b\chi^{-c}$ with $b = 0.335$ and $c = 1.994$, the critical point is estimated as $D_c = D_B(\infty) = 0.264$.

III. FIDELITY PER LATTICE SITE AND BIFURCATIONS

One can define a fidelity $F(D, D') = |\langle\Psi(D')|\Psi(D)\rangle|$ from a ground state wavefunction $\Psi(D)$. A fidelity per lattice site (FLS) d [16] can be defined as

$$\ln d(D, D') = \lim_{N\to\infty} \frac{\ln F(D, D')}{N}. \tag{3}$$

where N is the system size. Remarkably, FLS is well defined and plays a similar role to an order parameter although $F(D, D')$ trivially becomes zero in the thermodynamic limit when N approaches infinity. The FLS satisfies the properties inherited from fidelity $F(D, D')$: (i) normalization $d(D, D) = 1$, (ii) symmetry $d(D, D') = d(D', D)$, and (iii) range $0 \leq d(D, D') \leq 1$.

On adapting the transfer matrix approach [21], the iMPS representation of the ground-state wave-functions allows us to calculate the fidelity per lattice site (FLS)

$d(D, D')$. Let us choose $|\Psi(D')\rangle$ as a reference state for the FLS $d(D, D')$. For $D' = 0.26$, in Fig. 1, the FLS $d(D, D')$ is plotted as a function of the DM interaction parameter D for various values of the truncation dimensions with a randomly chosen initial state in the iMPS representation. Figure 1 shows a singular behavior of the FLS $d(D, 0.26)$, which indicates that there occurs a quantum phase transition across the singular point. A bifurcation behavior of the FLS $d(D, 0.26)$ is also shown when the interaction parameter D becomes smaller than its characteristic singular value that can be called a 'bifurcation point' D_B. The bifurcation points depend on the truncation dimension χ, i.e., $D_B = D_B(\chi)$. As the truncation dimension χ increases, the bifurcation occurs starting at the lower value of D. For $\chi \to \infty$, the bifurcation point $D_B(\infty)$ at which a bifurcation starts to occur can be extrapolated. In the inset of Fig. 1, we use an extrapolation function $D_B(\chi) = a + b\,\chi^{-c}$, characterized by the coefficients a, b, and c being a positive real number, which guarantees that $D_B(\infty)$ becomes a finite value. The numerical fitting gives $a = 0.264$, $b = 0.335$, and $c = 1.994$. From the extrapolation, the bifurcation point is shown to saturate to $D_B(\infty) \simeq a$ which can be regarded as a critical point $D_c = D_B(\infty)$ [22, 23]. Actually, the critical point also corresponds to the pinch point of the FLS in the thermodynamics limit, i.e., $\chi \to \infty$. Consequently, a FLS bifurcation point $D_B(\chi)$ plays the role of a pseudo phase transition point for a given finite truncation dimension χ in the MPS representation. In addition, the continuous function behavior of the FLS across the bifurcation point implies that a continuous quantum phase transition occurs at the critical point [16].

In Fig. 1, the bifurcation occurs for $D < D_B(\chi)$, which is captured in the iMPS representation with a randomly chosen initial state. In fact, the bifurcation behavior of the FLS means that there are two possible ground states for $D < D_B(\chi)$ while there is a single ground state for $D > D_B(\chi)$. Such a property of the ground states can be understood by the Z_2 symmetry of the Hamiltonian from the invariant transformation $UHU^\dagger = H$. In the thermodynamic limit, there are two possible ground states satisfying $UHU^\dagger = H$, that is, Ψ_g or $U\Psi_g$. Once a spontaneous symmetry breaking happens, the system can choose one of two possible ground states Ψ_g or $U\Psi_g$, which indicate a broken symmetry phase. For symmetric phase, the system has a single ground state, being a linear combination of two possible ground state, which should satisfy the transformation invariance. In Fig. 1, then, the FLS is plotted from the two fidelities, i.e., $F = |\langle\Psi_g(0.26)|\Psi_g(D)\rangle|$ (upper lines) and $F = |\langle\Psi_g(0.26)|U|\Psi_g(D)\rangle|$ (lower lines). Then, the bifurcation point is the transition point between the symmetry phase and the broken-symmetry phase.

IV. PHASE DIAGRAM

From the iMPS with the numerical extrapolation of the bifurcation points, in Fig. 2, we draw the ground-state phase diagram in the interaction parameter (r, D) plane. Below the phase boundary (red solid line) the system is in an antiferromagnetic phase while above the boundary the system is in a disordered phase. The phase diagram shows that the D_c is inversely proportional to the r_c. A best fitting function (dotted line) of the critical points (r_c, D_c) is given by $D_c \approx (a(a+1))/(\sqrt{r_c} + a) - a$ with a single parameter $a = 3.4$. The characteristic phase boundary can be understood as follows: If $r \neq 0$ and $D = 0$, the lattice sites are dimerised and the Hamiltonian in Eq. (1) has a two-site translational invariance due to the alternating bond coupling r. As assumed, for the antiferromagnetic exchange interaction $J_i > 0$, i.e., for $0 \leq r \leq 1$, the Ising chain with the alternating bond coupling is in an antiferromagnetic state even though the lattice sites are strongly dimerised. If $D \neq 0$, the antisymmetric anisotropic DM interaction can destroy the antiferromagnetic order originating from the antiferromagnetic exchange interaction J_i. The antiferromagnetic order may be destroyed more easily by the uniform antisymmetric anisotropic DM interaction for the dimerised lattice sites than for the Ising chain without the alternating bond coupling because the antiferromagnetic correlation between the sites becomes weaker due to the dimerised lattice sites. Then, to destroy the antiferromagnetic order, a stronger dimerisation of the lattice sites (bigger r) requires a much weaker uniform antisymmetric anisotropic interaction (much smaller D). Consequently, the phase boundary separating the antiferromagnetic phase and a disordered phase might have a inversely proportional relation between D_c and r_c.

Very recently, a real space renormalization group (RSRG) approach [24] has been applied in the same model and has shown that a symmetric phase boundary is given by $D_c \simeq \sqrt{1 - r_c^2}$ (blue dashed line in Fig. 2). Compared with the RSRG approach, our results from the iMPS show that there is a quite significant discrepancy in the phase boundary line because, contrast to the iMPS, the RSRG is an approximate method based on low-energy states, which implies that it does not capture properly a contribution from relevant higher energy states. Then, the ground state phase diagram from our fidelity approach based on the iMPS is more reliable and accurate.

V. QUANTUM ENTANGLEMENT AND PHASE TRANSITION

In order to understand more clearly the quantum phase transition in our system, let us consider quantum entanglement that can also detect a quantum phase transition [25]. To quantify the quantum entanglement, we employ the von Neumann entropy, which is a good measure

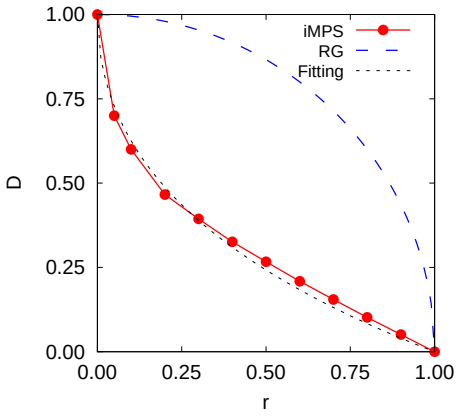

FIG. 2: (Color online) Ground state phase diagram in the plane of the DM interaction and the alternating bond strengths. From the iMPS, the phase boundary shows that the D_c is inversely proportional to the $\sqrt{r_c}$. A best fitting is denoted by the dotted line. This is in sharp contrast with the results from the real space renormolaztion group (RSRG) method [24].

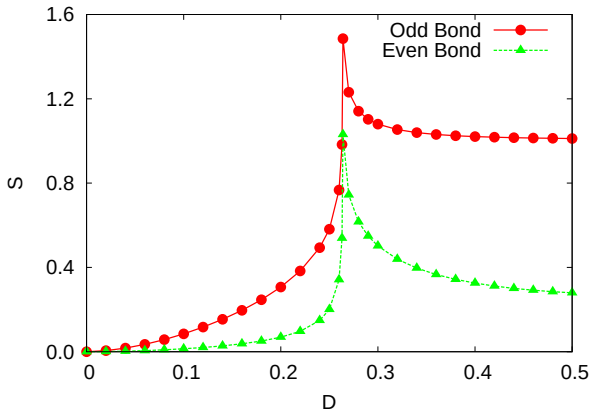

FIG. 3: (Color online) The von Neumann entropy S between left and right halves of a chain as a function of D for $r = 0.5$ and $\chi = 32$. Both the von Neumann entropies for odd and even bonds show a singularity at $D_c = 0.264$.

of bipartite entanglement between two subsystems of a pure state [26], because our ground states are in a pure state. Then, the spin chain can be partitioned into the two parts denoted by the left semi-infinite chain L and the right semi-infinite chain R. The von Neumann entropy is defined as $S = -\mathrm{Tr}\varrho_L \log_2 \varrho_L = -\mathrm{Tr}\varrho_R \log_2 \varrho_R$ in terms of the reduced density matrix ϱ_L or ρ_R of the subsystems L and R. In the iMPS representation, the von Neumann entropy for the semi-infinite chains L or R becomes

$$S_i = -\sum_{\alpha=1}^{\chi} \lambda_{i,\alpha}^2 \log_2 \lambda_{i,\alpha}^2, \tag{4}$$

where $\lambda_{i,\alpha}$'s are diagonal elements of the matrix λ that could be directly obtained in the iMPS algorithm. This is because, when one partitions the two semi-infinite chains $L(-\infty, \cdots, i)$ and $R(i+1, \cdots, \infty)$, one gets the Schmidt decomposition $|\Psi\rangle = \sum_{\alpha=1}^{\chi} \lambda_{i,\alpha} |\phi_L\rangle |\phi_R\rangle$. From the spectral decomposition, $\lambda_{i,\alpha}^2$ are actually eigenvalues of the reduced density matrices for the two semi-infinite chains L and R. In our two-site translational invariant iMPS representation, there are two Schmidt coefficient matrices λ_A and λ_B that describe two possible ways of the partitions, i.e., one is on the odd sites, the other is on the even sites. From the λ_A and λ_B, one can obtain the two von Neumann entropies depending on the odd- or even-site partitions.

In Fig. 3, we plot the von Neumann entropy S as a function of the DM interaction strength D for even ($2i$ site) and odd ($(2i+1)$ site) bonds with $r = 0.5$. The von Neumann entropy for the odd bonds is always larger than those for the even bonds because, by the definition, the odd-site exchange interaction J_{2i} is stronger that the even-site exchange interaction J_{2i+1}. Furthermore, it is shown that both the entropies for the even and odd bonds have a singularity at the same value of the DM interaction strength D. Note that the singularities of the entropies occur at the critical point $D_c = 0.264$. This result then shows clearly that both the FLS d and the von Neumann entropy S give the same phase transition point. As a consequence, in fact, the von Neumann entropy S gives the same phase diagram from the FLS in Fig. 2.

As discussed, for the antiferromagnetic state of our system, there are two possible ground states that are connected by the unitary transformation U. From the bifurcation of FLS, then, one might expect a bifurcation in the von Neumann entropy too. However, contrary to the FLS d, in Fig. 3, no bifurcation is seen in the von Neumann entropy S for the antiferromagnetic state even though the initial state is randomly chosen in the iMPS representation. The reason for the absence of bifurcation in the von Neumann entropy is why the singular values λ_i in Eq. (4) do not depend on the unitary transformation because the unitary transformation U acts only on a single site of the spin lattice in the iMPS representation.

VI. CENTRAL CHARGE AND UNIVERSALITY CLASS

At a critical point, characteristic singular behaviors of thermodynamics system properties depend only on few features such as dimensionality and symmetry, which can be classified by the concept of universality classes. Especially, the central charge can be used for the classification of universality classes [27, 28]. Owing to implement the iMPS representation, we can obtain a central charge c and a so-called finite-entanglement scaling exponent κ numerically via the unique behaviors of the correlation length ξ and the von Neumann entropy S with respect to the truncation dimension χ at a critical point [29, 30],

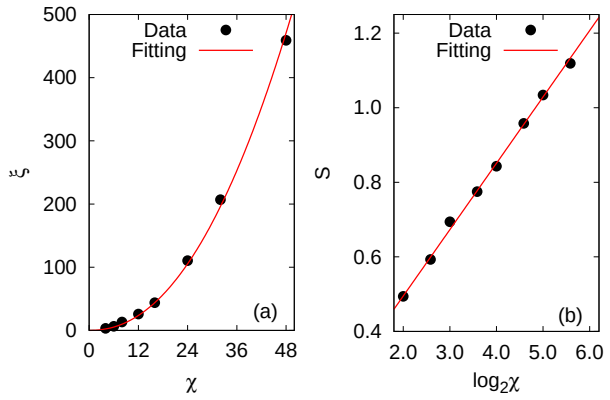

FIG. 4: (Color online) (a) Correlation length ξ as a function of the truncation dimension χ at the critical point. The power curve fitting $\xi = a\chi^{\kappa}$ yields $a = 0.112$ and $\kappa = 2.132$. (b) Scaling of the von Neumann entropy S with the truncation dimension χ at the critical point. For $\kappa = 2.132$ from (a), the linear fitting $S = (c\kappa/6)\log_2\chi + b$ yields the central charge $c \approx 0.494$. Here, the alternating bond strength is chosen as $r = 0.5$.

i.e.,

$$\xi = a\chi^{\kappa}, \tag{5}$$

$$S = \frac{c\kappa}{6}\log_2\chi. \tag{6}$$

In Fig. 4, the correlation length ξ and the von Neumann entropy S as a function of the truncation dimension χ at the critical point D_c for $r = 0.5$. Here, the truncation dimensions are taken as $\chi = 4, 6, 8, 12, 16, 24, 32,$ and 48. It is shown that both the correlation length ξ and the von Neumann entropy S diverges as the truncation dimension χ increases. From a power-law fitting on the correlation length ξ, we have $\kappa = 2.132$ and $a = 0.112$. As shown in Fig. 4 (b), our numerical result demonstrates a linear scaling behavior, which gives a central charge $c \simeq 0.494$ with $\kappa = 2.132$. Our central charge is close to the exact value $c = 1/2$. Consequently, the quantum phase transition in our system is in the same universality class as the quantum transverse field Ising model.

VII. SUMMARY

Quantum phase transitions have been investigated in the Ising chain with the Dzyaloshinskii-Moriya interaction as well as the alternating bond-coupling. The FLS and its bifurcation have clearly shown a characteristic singular point as a signature of the quantum phase transition and behaves as a continuous function, which shows a continuous phase transition occurring at the critical point. The phase diagram was obtained from the FLS and the von Neumann entropy. With a finite-entanglement scaling of the von Neumann entropy with respect to the truncation dimension in the iMPS representation, a central charge was estimated to be $c \simeq 0.5$, which shows that the system is in the same universality class with the quantum transverse field Ising model.

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